1-Hexanol, 3,3,4,4,5,5,6,6,6-nonafluoro-2043-47-2 | DTXSID1062122

2043-47-2 DTXSID1062122	

Model Performance

Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: 3.83

Global applicability domain: Inside

Local applicability domain index: 9.64e-01

Confidence level: 8.15e-01

Nearest Neighbors from the Training Set

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tert-Butyl alcohol Measured: 3.50 Predicted: 3.81 Image not found

2-Methyl-1-propanol Measured: 3.93 Predicted: 3.95 Image not found

2-Butanol Measured: 3.85 Predicted: 3.95

Image not found

1-Propanol Measured: 3.71 Predicted: 3.75 Image not found

2-Chloroethanol Measured: 4.30 Predicted: 4.07